

# Antisymmetrized molecular dynamics of wave packets with stochastic incorporation of Vlasov equation

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## Abstract

On the basis of the antisymmetrized molecular dynamics (AMD) of wave packets for the quantum system, a novel model (called AMD-V) is constructed by the stochastic incorporation of the diffusion and the deformation of wave packets which is calculated by Vlasov equation without any restriction on the one-body distribution. In other words, the stochastic branching process in molecular dynamics is formulated so that the instantaneous time evolution of the averaged one-body distribution is essentially equivalent to the solution of Vlasov equation. Furthermore, as usual molecular dynamics, AMD-V keeps the many-body correlation and can naturally describe the fluctuation among many channels of the reaction. It is demonstrated that the newly introduced process of AMD-V has drastic effects in heavy ion collisions of  $^{40}\text{Ca} + ^{40}\text{Ca}$  at 35 MeV/nucleon, especially on the fragmentation mechanism, and AMD-V reproduces the fragmentation data very well. Discussions are given on the interrelation among the frameworks of AMD, AMD-V and other microscopic models developed for the nuclear dynamics.

## I. INTRODUCTION

Heavy ion reactions in medium energy region give us opportunities to study the dynamics of the highly excited nuclear system far from the equilibrium and various kinds of theoretical models have been developed to describe the variety of phenomena realized in such reactions. There are many models which belong to the category of one-body transport models, such as the time-dependent Hartree Fock theory (TDHF). Vlasov equation [1] can be regarded as the semiclassical approximation of TDHF. In these models, the one-body distribution function for a Slater determinant propagates in the mean field which depends on itself. Vlasov-Uehling-Uhlenbeck (VUU) equation [2,3] includes the two-nucleon collision term as the effect of the residual interaction on the one-body distribution function. However, the description only with a one-body distribution function cannot be a good framework for the reaction system which has various final channels like fragmentation and therefore should be described by the linear combination of many Slater determinants in principle. When the one-body transport models are applied to such a system, the use of the averaged mean field common to all channels brings about spurious correlation among the time evolutions of channels which should be independent of one another in the true solution due to the linearity of the time-dependent Schrödinger equation.

On the other hand, molecular dynamics models [4–8] can be applied to the reaction system with many channels because they treat each channel as an independent event. Although the one-body transport model is an approximation of the molecular dynamics for point particles in the context of the classical dynamics, this relation is rather opposite for the quantum system in which any particle should have phase space distribution due to the uncertainty relation. In the antisymmetrized molecular dynamics (AMD) [8], for example, the system is described by a Slater determinant of Gaussian wave packets and the time evolution of the centroids of wave packets is determined by the equation of motion derived from the time-dependent variational principle. This equation of motion may be interpreted as an approximation of TDHF (or Vlasov) equation in the sense that TDHF gives better prediction of the instantaneous time evolution of an AMD wave function than AMD does because the TDHF single-particle wave function is more general than the AMD single-particle wave function. However, it should be noticed that this does not always mean that TDHF is superior to AMD in the global time scale, because AMD treats many channels and respects their independence, which is more important than the flexibility of single-particle wave functions for the system with many channels such as the multifragmentation. In AMD and many other molecular dynamics models, the branching process into channels is introduced by the stochastic collisions between two wave packets which correspond to the collision term in VUU equation but produce large fluctuation among events or channels. Therefore, even when we begin with a single initial state, many final channels are obtained by repeating the calculation. It is generally believed that molecular dynamics models can describe the fragmentation in heavy ion collisions.

Besides the two-nucleon collision process, there is another source of branching which is important even in low energy phenomena irrelevant to the two-nucleon collisions. A simple example can be found in the nucleon emission from a hot nucleus. When TDHF is applied to a hot fragment which has been produced in one of the channels of the true solution, a minor part of a single particle wave function will go out of the nucleus and the other

main part will remain in the nucleus unless the excitation energy is very large. Although TDHF will give good predictions of the emission probability and the nucleon spectrum, how reliable is the description of the residue nucleus? Depending on whether the nucleon has been emitted or not, the mean field of the residue nucleus should be made by  $A - 1$  nucleons or  $A$  nucleons respectively, but TDHF and other one-body transport models do not include such fluctuation between channels. Similar kind of fluctuation among channels is also important in the nucleon transfer in heavy ion collision, the fragment formation by the coalescence mechanism, and so on. In many cases when a single-particle wave function has spread wide or has splitted into several parts, the system should be branching into channels and therefore the TDHF description as a Slater determinant breaks down. In such cases, it seems better to decompose a Slater determinant into several Slater determinants and solve the later time evolution of each component independently.

On the other hand, in the molecular dynamics models with wave packets, the equation of motion chooses only the most important channel among the channels of the true solution if there is no source of fluctuation such as the stochastic two-nucleons collisions, though a variety of final channels are possibly generated in medium energy heavy ion collisions due to the fluctuation produced by the two-nucleon collisions. In our recent study of statistical property of AMD [9,10], we found that the ensemble of AMD wave functions of a hot nucleus has good statistical property of quantum mechanics in the observables such as the single-particle momentum distribution and the occupation probability of single-particle levels [10]. However, AMD has problem in the description of the future time evolution of the minor high-momentum component as an independent branch, which is the origin of the failure in the nucleon emission and the phase equilibrium of liquid and gas [9]. The minor branch of the nucleon emission which should be caused by the high-momentum tail is not respected at all in the dynamics and the whole nucleon wave packet remains in the nucleus because the wave packet is not allowed to split off. Therefore the ironical conclusion of the study of statistical property of AMD was that the problem is not due to anything very complex and uncontrollable by the usual microscopic considerations but due to the rather simple single-particle motion which has restriction in molecular dynamics with wave packets. This means in turn that we have chance to overcome this problem by respecting the spreading and the splitting of wave packets which are naturally predicted by simple one-body considerations. In fact, we showed in Ref. [9] that the problem of the nucleon emission can be solved by taking account of the stochastic splitting of the wave packet based on its momentum width when a nucleon wave packet is being emitted from the nuclear surface. It should be emphasized that with this stochastic method there is no spurious correlation of the above-mentioned TDHF calculation between channels with and without nucleon emission. However, in the dynamics of nuclear reactions, there may be other phenomena caused by the wave packet tail that are lost completely in AMD due to the restriction of the single-particle states.

The first purpose of this paper is to present an extended AMD model which can generally describe such minor branching processes by removing the restriction on the one-body distribution function. This is done not by generalizing the wave packets to arbitrary single-particle wave functions but by representing the diffused and/or deformed wave packet as an ensemble of Gaussian wave packets. In other words, stochastic displacements are given to the wave packets in phase space so that the ensemble-average of the time evolution of the one-body distribution function is essentially equivalent to the solution of Vlasov equation

which does not have any restriction on the shape of wave packets. This new model is called AMD-V. Although AMD-V is equivalent to Vlasov equation in the instantaneous time evolution of the one-body distribution function for an AMD wave function, AMD-V describes the branching into channels and the fluctuation of the mean field which are caused by the spreading or the splitting of the single-particle wave function. Furthermore, the stochastic two-nucleon collision process is included in AMD-V just in the same way as in AMD and other molecular dynamics models.

The second purpose of this paper is to show the drastic effect of this new stochastic process of wave packet splitting on the dynamics of heavy ion collisions, especially in the fragmentation mechanism. We take the  $^{40}\text{Ca} + ^{40}\text{Ca}$  system at the incident energy 35 MeV/nucleon. It will be shown that the reproduction of data by the AMD-V calculation is surprisingly good. From the previous study of the nucleon-emission process, it is automatically expected that the decay of the produced fragments should be too slow in AMD calculation, which will be proved in this paper by the comparison of AMD and AMD-V. However, the deviation between AMD and AMD-V appears not only in the decay of equilibrated fragments but also in early stages of the reaction. In fact, we will see that the effect of the wave packet diffusion is crucially important to remove the spurious binary feature of the AMD calculation and to enable the multi-fragment final state.

This paper is organized as follows. In Sec. II, the formulation of the new process of AMD-V is given in detail, and then in Sec. III, the calculated results of AMD and AMD-V are compared with each other and also with the experimental fragmentation data, to show the importance of the new process of AMD-V. Section IV is devoted to the discussion on the relation of AMD and AMD-V to other microscopic dynamical models such as TDHF and VUU. Summary is given in Sec. V.

## II. FORMULATION OF AMD-V

### A. Usual AMD

Before the incorporation of the stochastic process of wave packet splitting, we will explain the usual AMD [8] very briefly for the convenience of the readers. AMD describes the nuclear many body system by a Slater determinant of Gaussian wave packets as

$$\Phi(Z) = \det \left[ \exp \left\{ -\nu (\mathbf{r}_j - \mathbf{Z}_i / \sqrt{\nu})^2 + \frac{1}{2} \mathbf{Z}_i^2 \right\} \chi_{\alpha_i}(j) \right], \quad (1)$$

where the complex variables  $Z \equiv \{\mathbf{Z}_i\}$  are the centroids of the wave packets. We took the width parameter  $\nu = 0.16 \text{ fm}^{-2}$  and the spin isospin states  $\chi_{\alpha_i} = \text{p } \uparrow, \text{p } \downarrow, \text{n } \uparrow, \text{or n } \downarrow$ . The time evolution of  $Z$  is determined by the time-dependent variational principle and the two-nucleon collision process. The equation of motion for  $Z$  derived from the time-dependent variational principle is

$$i\hbar \sum_{j\tau} C_{i\sigma,j\tau} \frac{dZ_{j\tau}}{dt} = \frac{\partial \mathcal{H}}{\partial Z_{i\sigma}^*}. \quad (2)$$

$C_{i\sigma,j\tau}$  with  $\sigma, \tau = x, y, z$  is a hermitian matrix, and  $\mathcal{H}$  is the expectation value of the Hamiltonian after the subtraction of the spurious kinetic energy of the zero-point oscillation of the center-of-masses of fragments,

$$\mathcal{H}(Z) = \frac{\langle \Phi(Z) | H | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle} - \frac{3\hbar^2\nu}{2M}A + T_0(A - N_F(Z)), \quad (3)$$

where  $N_F(Z)$  is the fragment number, and  $T_0$  is  $3\hbar^2\nu/2M$  in principle but treated as a free parameter for the adjustment of the binding energies. Two-nucleon collisions are introduced by the use of the physical coordinates  $W = \{\mathbf{W}_i\}$  which are defined as

$$\mathbf{W}_i = \sum_{j=1}^A (\sqrt{Q})_{ij} \mathbf{Z}_j, \quad Q_{ij} = \frac{\partial \log \langle \Phi(Z) | \Phi(Z) \rangle}{\partial (\mathbf{Z}_i^* \cdot \mathbf{Z}_j)}. \quad (4)$$

## B. Stochastic incorporation of Vlasov equation

### 1. Basic idea

In molecular dynamics models with wave packets, each nucleon  $i$  at the time  $t = t_0$  is represented by a Gaussian wave packet in phase space

$$f_i(\mathbf{r}, \mathbf{p}, t_0) = 8 e^{-2\nu(\mathbf{r}-\mathbf{R}_i(t_0))^2 - (\mathbf{p}-\mathbf{P}_i(t_0))^2/2\hbar^2\nu}, \quad (5)$$

with the centroid  $\mathbf{R}_i$  and  $\mathbf{P}_i$ . This wave packet satisfies the minimum uncertainty relation. The total one-body distribution function  $f$  is the sum of  $f_i$ . In the case of AMD, this representation of each nucleon as a simple Gaussian wave packet is valid approximately if we use the physical coordinate

$$\mathbf{W}_i = \sqrt{\nu} \mathbf{R}_i + \frac{i}{2\hbar\sqrt{\nu}} \mathbf{P}_i \quad (6)$$

as the centroid. The time evolution of the centroids  $\dot{\mathbf{R}}_i$  and  $\dot{\mathbf{P}}_i$  are derived from the equation of motion while the shape of wave packets is fixed.

However, more reliable time evolution of the one-body distribution function is given by TDHF equation or Vlasov equation, which is the semiclassical approximation of TDHF equation,

$$\frac{\partial f_i}{\partial t} + \frac{\partial h}{\partial \mathbf{p}} \cdot \frac{\partial f_i}{\partial \mathbf{r}} - \frac{\partial h}{\partial \mathbf{r}} \cdot \frac{\partial f_i}{\partial \mathbf{p}} = 0, \quad (7)$$

where  $h = h(\mathbf{r}, \mathbf{p}, t)$  is the Wigner representation of the single-particle Hamiltonian calculated for the AMD wave function  $\Phi(Z(t_0))$  which is a Slater determinant. Although Vlasov (or TDHF) equation cannot give the reliable time evolution of the one-body distribution function in the situation where the system has branched into many channels like the fragmentation in heavy ion collisions, what we assume here is that the system is represented at  $t = t_0$  by an AMD wave function  $\Phi(Z(t_0))$  which is a Slater determinant of compact

single-particle wave functions, and therefore we can safely trust Vlasov equation for the instantaneous time evolution of the one-body distribution function.

In order to reflect Vlasov equation to AMD, we take the following stochastic procedure for each nucleon  $i$  during the short time step between  $t_0$  and  $t_0 + \delta t$ . For the simplicity of formulae, we introduce new notations

$$x = \{x_a\}_{a=1,\dots,6} = \{\sqrt{\nu} \mathbf{r}, \mathbf{p}/2\hbar\sqrt{\nu}\}, \quad (8)$$

$$X_i = \{X_{ia}\}_{a=1,\dots,6} = \{\mathbf{W}_i\} = \{\sqrt{\nu} \mathbf{R}_i, \mathbf{P}_i/2\hbar\sqrt{\nu}\}. \quad (9)$$

Then the one-body distribution function at  $t = t_0$  is represented as

$$f_i(x, t_0) = F(x - X_i(t_0)), \quad (10)$$

$$F(x) = \prod_{a=1}^6 \sqrt{2/\pi} e^{-2x_a^2}. \quad (11)$$

The essential point of AMD-V is to write the one-body distribution function at  $t = t_0 + \delta t$  as a superposition of Gaussian functions as

$$f_i(x, t_0 + \delta t) = (1 - c)F(x - X_i(t_0 + \delta t)) + c \int g(\xi)F(x - X_i(t_0 + \delta t) - \xi)d\xi, \quad (12)$$

with the integration variables  $\xi = \{\xi_a\}_{a=1,\dots,6}$ . Here we have introduced a parameter  $c$  and a normalized function  $g(\xi)$  which depend on  $\Phi(Z(t_0))$ ,  $\delta t$  and  $i$ . The case of  $c = 0$  corresponds to the usual AMD without shape changes of wave packets. If we allow arbitrary  $g(\xi)$  and  $c$ , it will be always possible to represent the exact solution of Vlasov equation. In order to enable the following prescription, it is further necessary to assume  $g(\xi) \geq 0$  and  $0 \leq c \leq 1$ . This restriction disables the description of the shrinking of the wave packet but seems reasonable since even under this restriction it is possible to describe the diffusion of the wave packet which is the important origin of the branching into channels but missing in the usual AMD. Let us assume that  $g(\xi)$  and  $c$  have been determined with a method given later so as to reproduce the solution of Vlasov equation as much as possible. Then it is possible to reflect Eq. (12) exactly within the framework of AMD by giving the stochastic displacement  $\xi$  with the probability  $c$  to the centroid of the wave packet according to the distribution function  $g(\xi)$ , together with the usual time evolution of the centroid by the equation of motion (and the stochastic two-nucleon collisions). It should be emphasized that the average value of the one-body distribution function after this stochastic process is just the same as Eq. (12) and the stochastic implementation is not an approximate treatment except for the restriction of  $g(\xi) \geq 0$  and  $0 \leq c \leq 1$ .

For the time step between  $t_0$  and  $t_0 + \delta t$ , the above-mentioned stochastic procedures are taken for all nucleons  $i$ . This means that the system has changed into an ensemble of many branches (or channels) at  $t_0 + \delta t$ , while it was a single Slater determinant at  $t_0$ . Each branch is represented by an AMD wave function and will make further branching in the following time steps just in the same way as was done at  $t_0$ . The future time evolution of each branch is solved without any influence from other branches. What is decisively important here is that the mean fields in  $\hbar$  are different from branch to branch, and therefore the fluctuation among channels are treated correctly unlike TDHF and other one-body transport models. This

situation is just the same as the branching caused by the stochastic two-nucleon collisions. In the practical calculation, only a path of branchings is followed in each simulation, and many simulations are repeated to get any observable which is calculated as the ensemble-average value of the expectation value all over the simulations.

## 2. Practical determination of the stochastic displacement

Now we explain a method to determine  $g(\xi)$  and  $c$  which we take in the calculation to be presented in this paper. Although there can be various methods, we take here the simplest method by taking account of only the dispersion of the wave packet

$$\sigma_{ab}^2(t) = \int (x_a - \bar{X}_a(t))(x_b - \bar{X}_b(t)) f_i(x, t) dx, \quad (13)$$

$$\bar{X}_a(t) = \int x_a f_i(x, t) dx, \quad (14)$$

where the dependence of  $\sigma_{ab}^2$  and  $\bar{X}_a$  on  $i$  should be understood implicitly. It should be noted that  $\sigma_{ab}^2(t = t_0) = (1/4)\delta_{ab}$ . The realistic time evolution of  $\sigma_{ab}^2$  can be obtained by Vlasov equation as

$$\dot{\sigma}_{ab}^2(t) \equiv \frac{d}{dt}\sigma_{ab}^2(t) = \int \left[ (\dot{x}_a - \dot{\bar{X}}_a(t))(x_b - \bar{X}_b(t)) + (x_a - \bar{X}_a(t))(\dot{x}_b - \dot{\bar{X}}_b(t)) \right] f_i(x, t) dx, \quad (15)$$

where  $\dot{x}$  is the solution of the classical equation of motion with the Hamiltonian  $h$  for the phase space point  $x$ ,

$$\{\dot{x}_a\} = \left\{ \sqrt{\nu} \dot{\mathbf{r}}, \dot{\mathbf{p}}/2\hbar\sqrt{\nu} \right\} = \left\{ \sqrt{\nu} \frac{\partial h}{\partial \mathbf{p}}, -\frac{\partial h}{\partial \mathbf{r}}/2\hbar\sqrt{\nu} \right\}, \quad (16)$$

and

$$\dot{\bar{X}}_a(t) = \int \dot{x}_a f_i(x, t) dx. \quad (17)$$

We can calculate  $\dot{\sigma}_{ab}^2(t_0)$  using the Monte Carlo integration method or the test particle method as is usually done in solving Vlasov equation for heavy ion collisions. Since  $\dot{\sigma}_{ab}^2(t_0)$  can be diagonalized by an orthogonal transformation, we can assume without losing generality that

$$\dot{\sigma}_{ab}^2(t_0) = \dot{\sigma}_a^2 \delta_{ab}. \quad (18)$$

It can be easily proved that

$$\text{Tr}[\dot{\sigma}_{ab}^2(t_0)] = \sum_{a=1}^6 \dot{\sigma}_a^2 = 0, \quad (19)$$

for the Gaussian wave packet  $f_i(x, t_0)$ . This relation can be considered as a representation of the Liouville theorem. In numerical calculations we find that three of  $\{\dot{\sigma}_a^2\}_{a=1,\dots,6}$  are

positive and three of them are negative in most cases. As we have mentioned before, we cannot treat the shrinking components but we respect the diffusing components by giving the stochastic displacement. Assuming that the reproduction of the second moment  $\dot{\sigma}_a^2$  of the diffusion is the most important and the effect of the higher moments is negligible, we take the distribution function of the stochastic displacement  $g(\xi)$  to have a deformed Gaussian form as

$$g(\xi) = \prod_{a; \dot{\sigma}_a^2 > 0} \sqrt{2\alpha_a/\pi} e^{-2\alpha_a \xi_a^2} \prod_{a; \dot{\sigma}_a^2 \leq 0} \delta(\xi_a), \quad (20)$$

$$\alpha_a = s^2/\dot{\sigma}_a^2, \quad s^2 = \frac{1}{6} \sum_{b=1}^6 |\dot{\sigma}_b^2|, \quad (21)$$

where  $s^2$  can be arbitrary but taken as above so that the typical width of  $g(\xi)$  is the same as that of the original wave packet  $f_i(x, t_0)$ . Then it is easily proved that  $\dot{\sigma}_{ab}^2(t_0)$  given by Vlasov equation are reproduced exactly by the stochastic displacement for the diffusing directions in phase space if we take the probability

$$c = 4s^2\delta t. \quad (22)$$

The choice of  $s^2$  is rather arbitrary because frequent small fluctuations and rare large fluctuations give the same diffusion effect  $\dot{\sigma}^2$ . Although it is also possible to take  $c = 1$  and  $\alpha_a = (4\dot{\sigma}_a^2\delta t)^{-1}$  for example, we take the above choice because the numerical calculation is easy when the probability  $c$  is small.

One may naively think that the above treatment of only the second moment of the diffusion by the Gaussian stochastic displacement were similar to the fermionic molecular dynamics (FMD) [7] which treats the widths of wave packets as dynamical variables. It is true only for the instantaneous time evolution of the one-body distribution function. The essential point of AMD-V is that each component of the diffused wave packet can propagate independently of other components and therefore it is allowed for the branched wave packets to evolve on completely different trajectories. This feature is very important in the nucleon emission process, for example, where the emitted (high-momentum) component and the low-momentum component remaining in the nucleus evolve in their own ways, while in FMD these two components influence each other in a complex way because of the nonlinearity of the approximate treatment of FMD.

### 3. Recovery of the conservation laws

The simple-minded stochastic displacement explained above brings about the violation of conservation laws such as the total momentum and the energy, and therefore the obtained final states cannot be interpreted as physically meaningful final channels of the reaction.

The problem of the momentum conservation is rather trivial. By the chain clustering method, we first define the nucleus that includes the nucleon  $i$  to which the stochastic displacement is to be given. Any pair of two nucleons  $j$  and  $k$  with  $|\mathbf{W}_j - \mathbf{W}_k| < 1.25$  is considered to belong to the same nucleus and the mass number of the nucleus which includes the nucleon  $i$  is denoted by  $A_{\text{nuc}}$ , excluding the nucleon  $i$ . The conservation law of the total



momentum of this nucleus means that the fluctuation of the single-particle momentum of the nucleon  $i$  should be compensated coherently by the other nucleons in this nucleus, though this correlation cannot be described by the single-particle models. Therefore, to respect the momentum conservation, we give the stochastic displacement  $\xi$  not to  $\mathbf{W}_i$  but to the relative coordinate

$$\mathbf{W}_i - \frac{1}{A_{\text{nuc}}} \sum_{j \in \text{nuc}} \mathbf{W}_j. \quad (23)$$

The conservation of the total energy should be considered more carefully. The branching by the stochastic process corresponds to the decomposition of a Slater determinant to a superposition of Slater determinants in the truly quantum mechanical description. Due to the interference among the Slater determinants, they need not to be the eigenstates of the energy in order for the total wave function to have the definite energy. However, while they are evolving in time toward the final channels of the reaction, their energies become the same as the initial energy, because the matrix elements of the Hamiltonian between different final channels are vanishing. In other words, the energy deviation of each Slater determinant produced by the stochastic displacement of a nucleon wave packet will be compensated by other degrees of freedom of the nucleus before the system reaches the final state. The standpoint of AMD-V is to respect the fluctuation and the independence among the channels at the cost of the interference among them. We neglect the finite time to recover the energy conservation and require that the energy should be conserved just after the stochastic displacement by adjusting other degrees of freedom of the nucleus. Now the problem is how to decide the way of the energy adjustment. The most natural requirement is that the energy conservation should be achieved with the least modification of the internal (canonical) coordinates of  $A_{\text{nuc}}$  nucleons in the nucleus that includes the nucleon  $i$  to which the stochastic displacement has been given now. For this purpose, we solve the constrained cooling/heating equation [11]

$$\mp \hbar \sum_{j\tau} C_{k\sigma,j\tau} \frac{dZ_{j\tau}}{d\beta} = \frac{\partial \mathcal{H}}{\partial Z_{k\sigma}^*} + \sum_{l=1}^n \eta_l \frac{\partial G_l}{\partial Z_{k\sigma}^*}, \quad (24)$$

until the energy becomes equal to the initial value with a reasonable precision. Here we have introduced several real functions  $\{G_l(Z)\}_{l=1,\dots,n}$  of the constraints which include the displaced coordinate  $\mathbf{W}_i$  of the nucleon  $i$ , the center-of-mass coordinate of  $A_{\text{nuc}}$  nucleons  $\sum_{j \in \text{nuc}} \mathbf{W}_j / A_{\text{nuc}}$ , and the coordinates of irrelevant nucleons which do not belong to the nucleus that includes the nucleon  $i$ . The Lagrange multipliers  $\{\eta_l\}$  should be determined so that the constraints are kept,  $dG_l/d\beta = 0$ . We further require that the energy adjustment should not change collective coordinates and include following constraint functions into  $\{G_l\}$ ,

$$\frac{\langle \Phi(Z) | \sum_k \mathbf{r}_k \times \mathbf{p}_k | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle} \quad (25)$$

and

$$\frac{\langle \Phi(Z) | \sum_k r_{k\sigma} r_{k\tau} | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle}, \quad \frac{\langle \Phi(Z) | \sum_k p_{k\sigma} p_{k\tau} | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle}, \quad (26)$$

with  $\sigma, \tau = x, y, z$ . These constraints of collective coordinates are based on the idea that the collective energy, such as the incident energy in heavy ion collisions, should not be converted directly to the energy for the stochastic displacement which arises from the independent single-particle motions.

One might have the opinion that it is not necessary to conserve the total energy because the AMD wave function  $\Phi(Z)$  is not an energy eigenstate. However, in the calculation of the nuclear reactions, the initial state is almost an energy eigenstate because AMD can describe the ground states of nuclei very well. As a matter of course, this small energy dispersion should be kept constant through the reaction in the exact solution. The reason why the AMD states  $\Phi(Z)$  during the reaction have large energy dispersion is not because it is physical situation but because the AMD functional space is limited so that all (thermally) excited states in AMD inevitably have large energy dispersion. Therefore it is not appropriate to take the energy dispersion of the AMD state as the physical one. It is rather reasonable to neglect this spurious energy dispersion in the procedure for the recovery of the energy conservation as explained above.

#### *4. Treatment of exceptional situations*

There are two kinds of exceptional (but frequently happening) situations in which the procedures described above do not go straight and the special care is required.

The first possibility is that the state  $W$  after the stochastic displacement is Pauli-forbidden [8] and there is no corresponding AMD wave function  $\Phi(Z)$ . Should we cancel this stochastic displacement like the Pauli-blocking in the two-nucleon collision process, or should we try again by generating another random number for the displacement? In order to answer this question, we first note that Vlasov equation already respects the Pauli principle in a semiclassical manner because the Liouville theorem in the classical dynamics ensures that  $f(\mathbf{r}, \mathbf{p}, t) \leq 1$  is satisfied for any  $t$  if the initial state satisfies the semiclassical Pauli principle  $f(\mathbf{r}, \mathbf{p}, t_0) \leq 1$  for each spin-isospin state. Since the stochastic displacement has been decided by the time evolution of  $f$  according to Vlasov equation, no further consideration of the Pauli principle is necessary. The state  $W$  after the stochastic displacement can be Pauli-forbidden because of the mismatch between the exact quantum treatment of the Pauli principle in AMD and the approximate semiclassical treatment in Vlasov equation. If we simply canceled the stochastic displacement, the correct diffusion given by Eq. (15) would not be obtained. Therefore, in the case of Pauli-forbidden  $W$ , we should try again by generating another random number for the stochastic displacement.

The second possibility is that the energy conservation is not achieved by solving Eq. (24) even when the system has cooled down to the energy minimum state under the given constraints. Should we cancel this stochastic process or try again by generating another value of the stochastic displacement? This situation often happens in the nucleus with low excitation energy and always in the ground state. One of the origin of this case is the mismatch between the quantum mechanics in AMD (or in TDHF) and the semiclassical treatment in Vlasov equation. The quantum one-body distribution function in AMD (or TDHF) has high-momentum component even for the bound states such as the ground state. Since we put this one-body distribution function into Vlasov equation as the initial state at

$t = t_0$ , the high-momentum component begins to go out of the nucleus and contributes to the diffusion calculated by Eq. (15), which should not happen if we treat quantum mechanically. Another origin of the impossible energy recovery is the mismatch between the many-body treatment in AMD and the averaged one-body treatment in Vlasov (or TDHF) equation. For example, if the excitation energy of the nucleus is less than the nucleon separation energy, no nucleon emission is possible in AMD due to the energy conservation. However, in Vlasov (or TDHF) equation, some part of a nucleon can go out without violating the conservation of the averaged energy. Since the energy of each branch (with or without nucleon emission) should be the same as the initial energy, the result of Vlasov (or TDHF) equation is unsatisfactory. From these consideration, we can say that the diffusion of the wave packet that cause the impossible energy recovery is spurious and should not have been included in Eq. (15) based on which this stochastic displacement is being considered. Therefore we should cancel this stochastic displacement rather than try again.

In summary, in order to fix the mismatches between AMD and Vlasov equation, the probability  $c$  and the distribution function  $g(\xi)$  of the stochastic displacement have been modified to  $c'$  and  $g'(\xi)$ ,

$$c' = c \frac{\int \Theta_E(X_i + \eta) \Theta_P(X_i + \eta) g(\eta) d\eta}{\int \Theta_P(X_i + \eta) g(\eta) d\eta}, \quad (27)$$

$$g'(\xi) = \frac{\Theta_E(X_i + \xi) \Theta_P(X_i + \xi) g(\xi)}{\int \Theta_E(X_i + \eta) \Theta_P(X_i + \eta) g(\eta) d\eta}, \quad (28)$$

with step functions of phase space point  $x$ ,

$$\Theta_P(x) = \begin{cases} 1 & \text{if } x \text{ is Pauli-allowed,} \\ 0 & \text{if } x \text{ is Pauli-forbidden.} \end{cases} \quad (29)$$

$$\Theta_E(x) = \begin{cases} 1 & \text{if energy adjustment is possible,} \\ 0 & \text{if energy adjustment is impossible.} \end{cases} \quad (30)$$

### III. APPLICATION TO HEAVY ION COLLISIONS

In this section, we will show the calculated results of  $^{40}\text{Ca} + ^{40}\text{Ca}$  reaction at 35 MeV/nucleon with AMD and AMD-V in order to demonstrate the importance of the newly introduced stochastic process of AMD-V to take account of the diffusion and the splitting of wave packets according to Vlasov equation.

In Ref. [12], this reaction system was analyzed with various models, including the quantum molecular dynamics (QMD) [6], the statistical sequential decay model (GEMINI) [13], and the simultaneous multifragmentation model of Gross [14]. None of these models reproduces the  $\alpha$  particle multiplicity  $M_\alpha$  which is as large as 5.2. Most models underestimate  $M_\alpha$  by a factor more than 2, while they overestimate the proton multiplicity  $M_p$  which is 6.2 in experiment. Although the microscopic dynamical calculation of QMD gives better result of the charge distribution of intermediate mass fragments (IMFs) than the other statistical

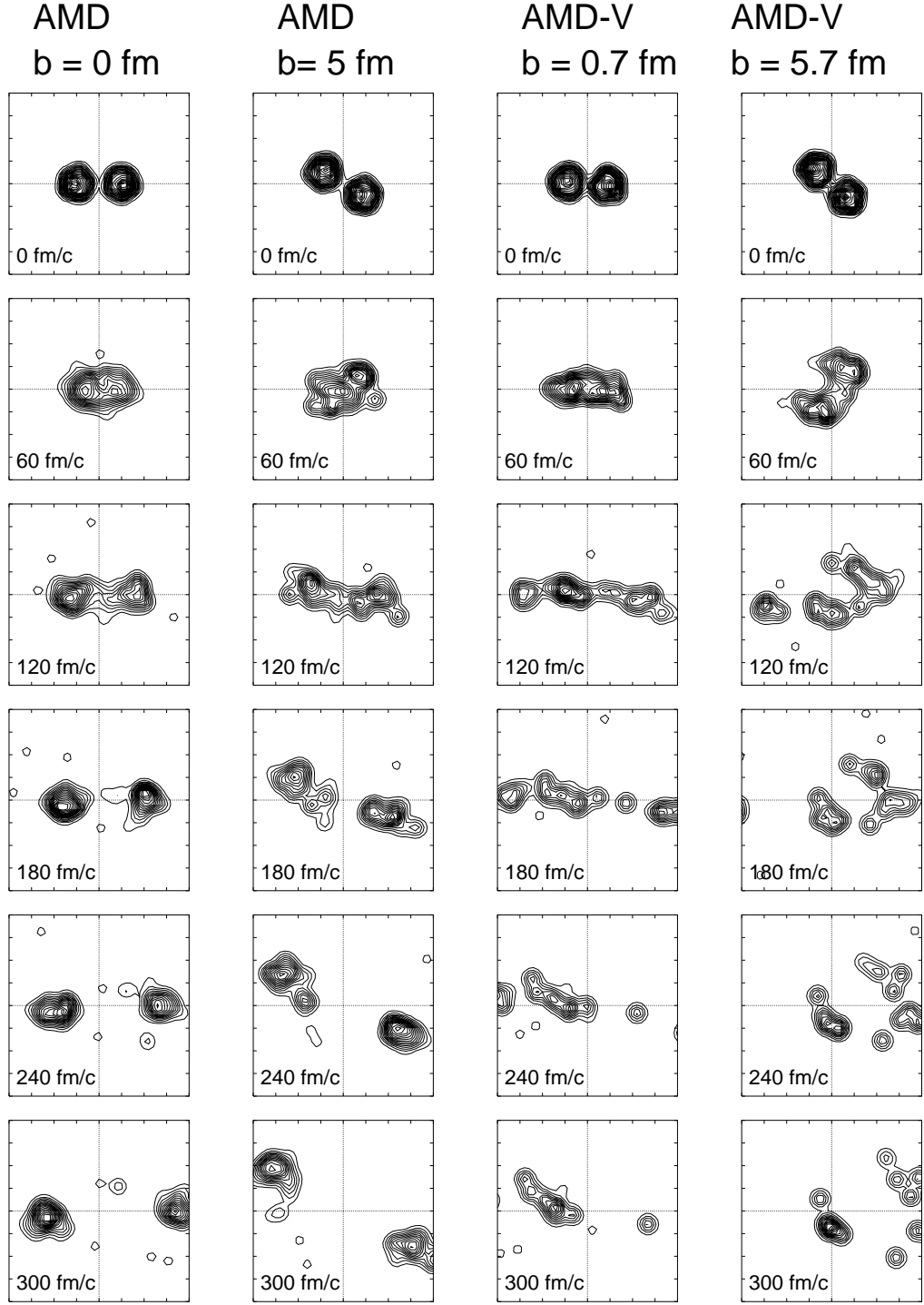


FIG. 1. Examples of the time evolution of the density projected onto the reaction plane from  $t = 0$  fm/c to  $t = 300$  fm/c for  $^{40}\text{Ca} + ^{40}\text{Ca}$  collisions at 35 MeV/nucleon. The size of the shown area is  $40\text{ fm} \times 40\text{ fm}$ . Calculated results with AMD (left two columns) and with AMD-V (right two columns) are shown for impact parameters  $b \sim 0$  fm and  $b \sim 5$  fm.

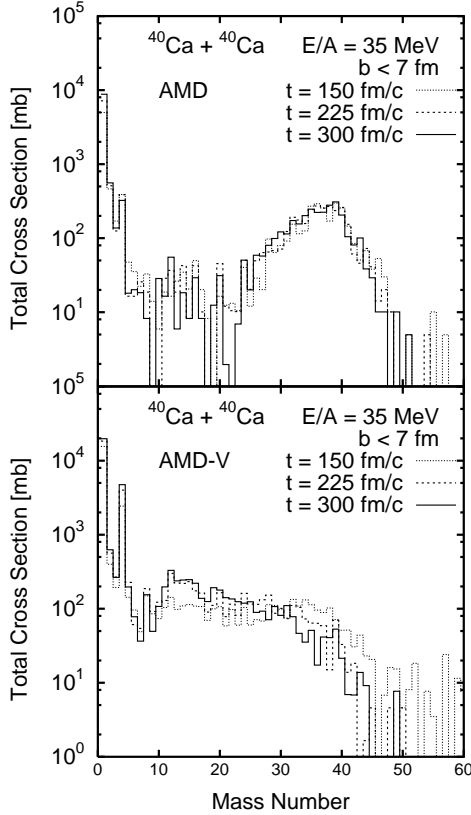


FIG. 2. Mass distribution of fragments that exist at  $t = 150$ ,  $225$ , and  $300$  fm/c in the dynamical calculations with AMD (upper part) and AMD-V (lower part).

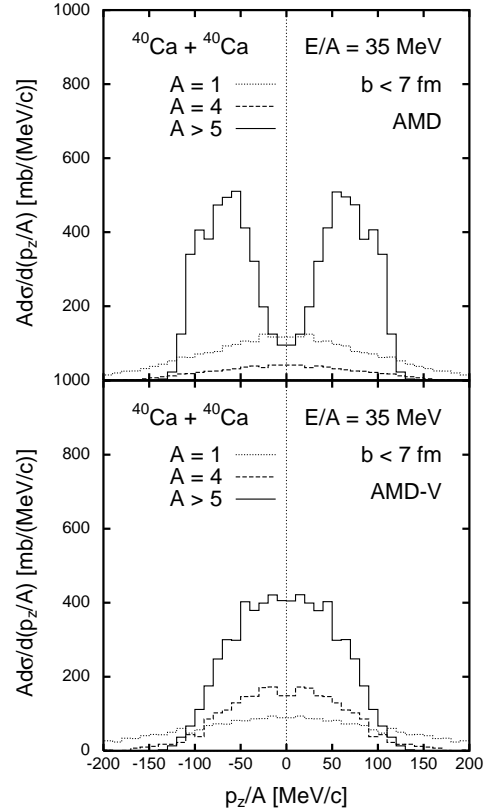


FIG. 3. Parallel momentum distribution of nucleons,  $\alpha$  particles and heavier fragments after the statistical decay calculated with AMD (upper part) and AMD-V (lower part). The vertical scale is proportional to the number of nucleons contained in the fragments. Incident momenta of the projectile and the target correspond to  $p_z/A = \pm 128$  MeV/c.

models, the unsatisfactory point is that the QMD dynamical calculation should be truncated early at  $t \sim 100$  fm/c and should be connected to a statistical decay model such as GEMINI in order to get good results. This means that the microscopic dynamical QMD calculation cannot describe the whole stage of the reaction consistently. It should be commented here that in the QMD used in Ref. [12] the kinetic energy does not include the zero-point oscillation energy though the density is the sum of Gaussian wave packets, and hence the extension formulated in the previous section is not directly applicable to this QMD.

The calculations with AMD and AMD-V are performed as usual. Gogny force [15] is adopted as the effective interaction. Coulomb force is included. The width parameter is taken to be  $\nu = 0.16$  fm $^{-2}$ . Two-nucleon collision cross section is the same as that used in Ref. [16]. It should be noted that there is no parameter introduced for the new stochastic process of AMD-V. Many simulations are repeated because each simulation corresponds to

an experimental event. The impact parameter region  $b < 7$  fm is investigated in this paper. Each dynamical simulation is continued until  $t = 300$  fm/c. The statistical decay of the excited fragments which exist at  $t = 300$  fm/c is calculated with a code [6] which is similar to CASCADE by Pühlhofer [17]. Although it is originally an evaporation calculation code, we take account of the sequential binary decay of a parent nucleus into two daughter nuclei both of which may be excited. The excitation energy of the lighter daughter nucleus is limited to  $E^* < 40$  MeV.

We first describe the features of the calculated results of the usual AMD. Left two columns of Fig. 1 show examples of the time evolution of the density projected onto the reaction plane. We can see that the projectile and the target pass through each other for both impact parameters  $b = 0$  fm and  $b = 5$  fm. This is generally true not only for these two events as can be seen in the upper part of Fig. 2 which shows the mass distribution of the fragments that exist at  $t = 150, 225$ , and  $300$  fm/c. There is a large peak around  $30 \lesssim A \lesssim 40$  which is contributed by the projectilelike and targetlike fragments in binary events. At  $t = 150$  fm/c, the system has already been separated into two large fragments and the later time dependence of the mass distribution is rather gradual. There is almost no yield for light IMFs with  $10 \lesssim A \lesssim 20$  in dynamical AMD calculation. The binary feature can be found not only in the mass distribution but also in the momentum distribution of fragments. Figure 3 shows the distribution of the momentum component parallel to the beam direction for particles with  $A = 1$ ,  $A = 4$ , and  $A > 5$  after the statistical decay calculation. For fragments with  $A > 5$ , the projectilelike and targetlike components are clearly separated into two peaks which have been largely shifted and dissipated from the incident values. Figure 4 shows the time-dependence of the internal energy of the matter part of the system which is defined as

$$(E/A)_{\text{matter}} = \sum_{k; A_k \geq 5} E_k / \sum_{k; A_k \geq 5} A_k, \quad (31)$$

where  $k$  is the label of the fragments that exist at the given time  $t$  in all events.  $A_k$  and  $E_k$  are the mass number and the internal energy of the fragment respectively, and the sum is taken for fragments with  $A_k \geq 5$ . As shown in the figure, the excitation energy of the two large fragments produced in AMD calculation is very high. If the ground state energy is assumed to be  $-7$  or  $-8$  MeV/nucleon, the averaged excitation energy of the fragments is about 5 MeV/nucleon. Furthermore, in spite of this very high excitation, the cooling of the fragments is very slow. It will take a time of order of 1000 fm/c for the fragments to lose 1 MeV/nucleon of the excitation energy if the AMD calculation is continued for a long time. When the decay of these fragments is calculated by the statistical decay code, they emit many nucleons and other light particles and the mass distribution of fragments changes largely as shown in the upper part of Fig. 5. The peak of the projectilelike and targetlike fragments has shifted to left by about 15. Reflecting the mass distribution before the statistical decay, there is a dip in the IMF region of  $10 \lesssim A \lesssim 20$ . The yields of  $\alpha$  particles and light IMFs have increased very much by the statistical decay process as well as the nucleon yield. In the case of  $\alpha$  particles, only 15 % of the final yield is due to the  $\alpha$  particles produced in the AMD calculation which is continued until  $t = 300$  fm/c. It should be noted that the fall of the yield for  $A \gtrsim 25$  is due to the finite impact parameter range  $b < 7$  fm.

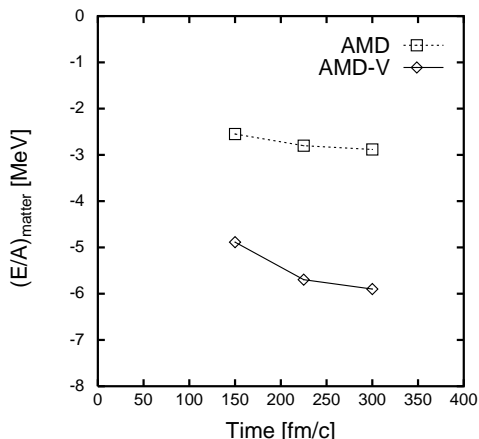


FIG. 4. Internal energy per nucleon of the matter part of the system (see text) in events with  $b < 5$  fm as a function of the time in the dynamical calculation of AMD (squares) and AMD-V (diamonds).

The features of the usual AMD calculation are summarized as follows: Reaction is almost always binary, and produced fragments are highly excited but their decay is very slow. Only few  $\alpha$  particles and light IMFs are produced in the dynamical stage of the reaction, though they can be produced by the statistical decay process. We do not think these features are realistic as explained below.

On the very slow deexcitation of fragments, we have already discussed in Refs. [9,10]. Namely the usual AMD should underestimate the nucleon emission rate from a hot nucleus because the momentum distribution of the nucleon wave packet is not duely reflected in the nucleon emission dynamics. In AMD, a nucleon cannot go out of the nucleus unless the wave packet centroid can go out of the nucleus, even though there should be some probability of nucleon emission due to the high-momentum tail of the wave packet. Even when a nucleon is emitted from the nucleus, the kinetic energy carried out by the emitted nucleon will be very small as also shown in Ref. [9] as the classical caloric curve. It should be noted that the wave packet spread in AMD is a very important factor for the nucleon emission because the energy spread due to the wave packet spread is  $3\hbar^2\nu/2M = 10$  MeV per wave packet. Therefore the usual AMD should be severely underestimating the nucleon emission rate from the excited fragments. This point can be improved by AMD-MF proposed in Ref. [9]. In AMD-MF, a stochastic fluctuation is given to the momentum centroid of a nucleon according to the momentum width of the wave packet when it is going out of the nucleus. By this method, the wave packet near the nuclear surface is allowed to split into several branches such as the high-momentum component and the low momentum component, and the high-momentum component can go out of the nucleus with a reasonable probability. This improvement is already contained in AMD-V which is a much more general framework than AMD-MF. According to Vlasov equation, the nucleon wave packet which is attacking the nuclear surface should change its shape in phase space because the high-momentum component begins to go out of the nucleus while the low-momentum component is reflected by the nuclear surface. Since this diffusion effect according to Vlasov equation is treated by AMD-V exactly, the nucleon emission is described reliably. In other words, the stochastic displacement is given to the wave packet centroid so that the wave packet is shifted to a high-momentum and outer-located value with a reasonable probability and then it can go

out of the nucleus.

The diffusion and the splitting of the wave packet should also affect the binary feature of the reaction. It should be noted that the wave packet centroids in the projectile or the target distribute in rather compact region of phase space compared to the nucleon distribution which is calculated as the centroid distribution folded by the width of each wave packet. Therefore, even when the projectile density and the target density overlap each other, the centroid distributions do not overlap in peripheral collisions. In the true solution, the nucleon transfer and/or the formation of participant hot region may happen in the overlapped region. However, these phenomena are impossible in AMD because the centroids in the projectile are passing far from the target in peripheral collisions, even though there should be some probability of nucleon transfer due to the tail component of the wave packet density distribution. Furthermore, the wave packet centroids in the two nuclei are well separated not only in the coordinate space but also in the momentum space, and therefore the spurious binary feature appears also in central collisions. The two-nucleon collisions which happen in AMD calculation do not help to remove the spurious binary feature, because most nucleons that are scattered by two-nucleon collisions are simply emitted as single nucleons.

Now let us turn to the results of AMD-V. The results have been shown in Figs. 1–5 together with the results of the usual AMD. With the introduction of the stochastic branching process based on the wave packet diffusion by Vlasov equation, the calculated results of the fragmentation have changed drastically. As can be seen in Fig. 1, the reaction is not binary any more. The dissipation of the incident energy is large but not complete (Fig. 3). Sometimes an elongated part is formed connecting the projectilelike and the targetlike parts in the intermediate stage of the reaction and a fragment can be left around the center-of-mass position in many events. This fragmentation mechanism seems to correspond to the interpretation of the neck fragmentation from the experimental analysis by Montoya et al. [18] As shown in Fig. 2, the yield of light IMFs with  $10 \lesssim A \lesssim 20$  has increased drastically compared to the case of the usual AMD. Most light IMFs are produced before  $t = 225$  fm/c. It should be also noticed that the yield of  $\alpha$  particles which are produced in the dynamical calculation is more than 10 times as large as in the usual AMD calculation. Dynamically emitted nucleons are twice as many as in the usual AMD. Although the system has been partitioned into smaller pieces, the produced fragments are much less excited as shown in Fig. 4. The excitation energy is only about 2 MeV/nucleon when a fragment is produced, and its deexcitation is more rapid than in the usual AMD. Since the excitation energies of the fragments at the end of the AMD-V calculation are already small, the statistical decay calculation has only a small effect on the mass distribution as shown in Fig. 5. It should be noted that the final yield of nucleons is slightly smaller than in the usual AMD, while the final yield of  $\alpha$  particles is much larger reflecting the large yield of the dynamically produced  $\alpha$  particles. The final mass distribution of IMFs is very different from that of the usual AMD.

In order to compare the calculated results by AMD and AMD-V with the experimental data [12], it is necessary to apply the experimental filter. In experiment, only the completely detected violent events are used for the analysis by selecting the events with the detected total charge  $Z_{\text{tot}} \geq 34$  and the detected charged particle multiplicity  $M_c \gtrsim 10$ . In the code of the experimental filter, the arrangement of the detectors and their thresholds are taken into account. In Fig. 6, the calculated charge distribution of fragments after the application of the



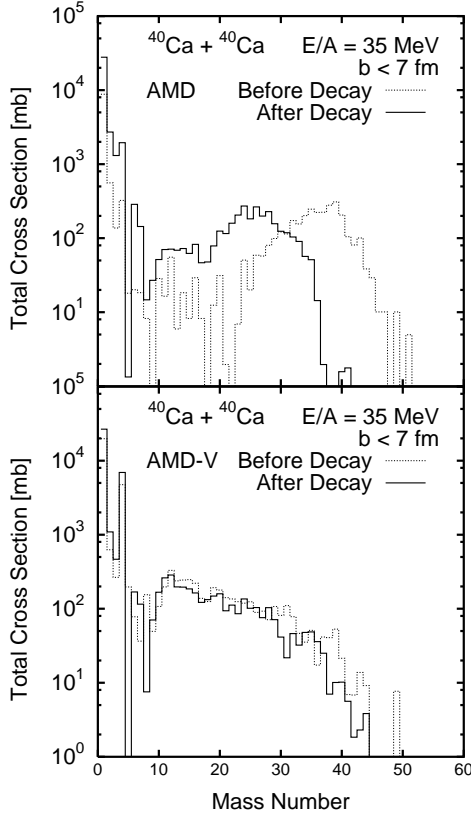


FIG. 5. Fragment mass distribution at the end of the dynamical calculation (dotted histogram) and after the statistical decay calculation (solid histogram). Results of AMD (upper part) and AMD-V (lower part) are shown.

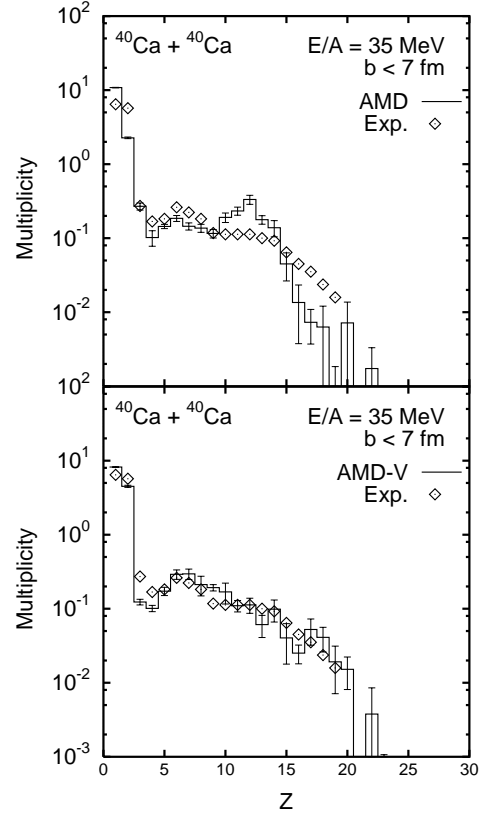


FIG. 6. Calculated charge distribution (histogram) compared with the experimental data (diamonds). The experimental filter has been applied. Error bars show the estimated statistical error of the calculated results. Results of AMD (upper part) and AMD-V (lower part) are shown.

experimental filter is compared with the data. We can see that the result of the usual AMD is not good while the result of AMD-V is quite satisfactory. However, the underestimation of the light IMF yield by the usual AMD is not so severe as could be expected from the inclusive mass distribution in Fig. 5. This is because of the experimental filter. Due to the high detector threshold, the targetlike fragments in the binary events are seldom detected and therefore most of the binary events are rejected by the experimental filter. On the other hand, the small number of ternary events are relatively favored by the experimental filter. Therefore the filtered result of the usual AMD does not reflect the feature of the total events correctly, but the binary feature is still left in the filtered charge distribution which is in contradiction to the data. The overestimation of the proton multiplicity  $M_p$  and the underestimation of  $\alpha$  multiplicity  $M_\alpha$  are common to other model calculations reported in Ref. [12]. On the other hand, AMD-V reproduces the charge distribution of fragments with  $Z \geq 5$  almost perfectly, which demonstrates strongly the ability of AMD-V to describe the fragmentation. Furthermore AMD-V has improved the problem of  $M_p$  and  $M_\alpha$  so much that

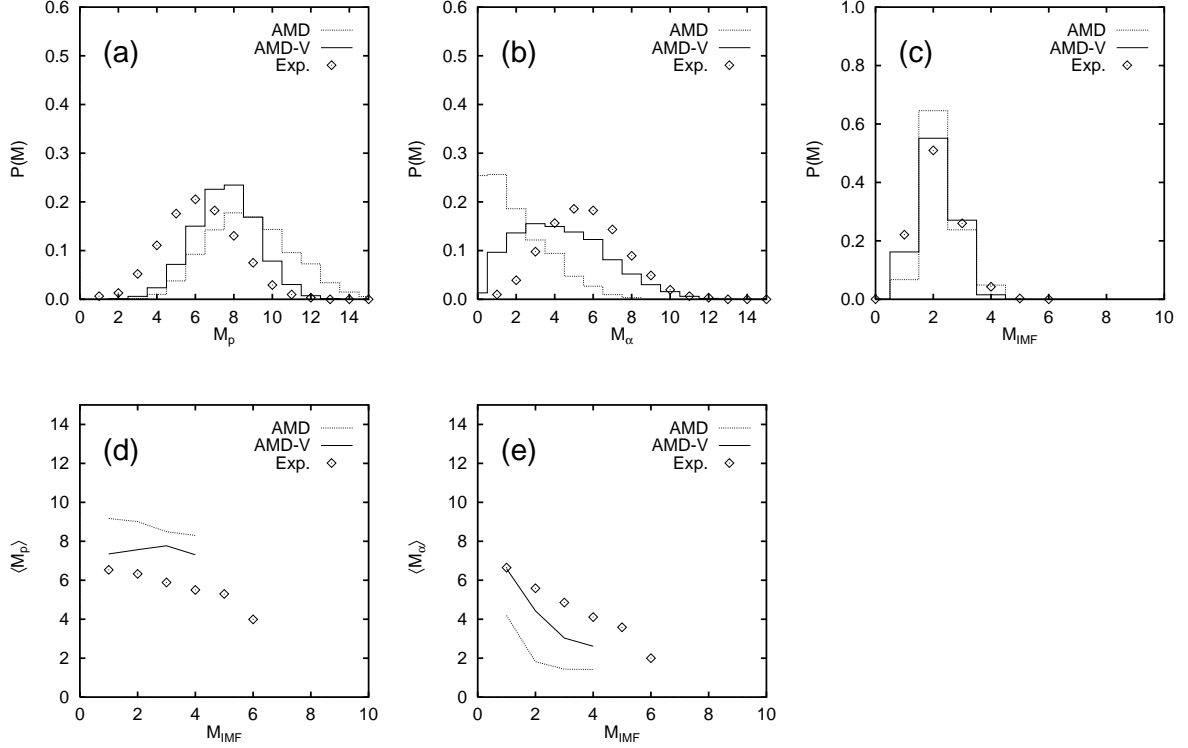


FIG. 7. Multiplicities of various products. Diamonds represent the experimental data, dotted lines represent the results of AMD, and solid lines represent the results of AMD-V. The experimental filter has been applied. (a) Proton multiplicity, (b)  $\alpha$  particle multiplicity, (c) IMF multiplicity, (d) proton multiplicity vs IMF multiplicity, and (e)  $\alpha$  particle multiplicity vs IMF multiplicity. In (d) and (e), calculated results are not shown for  $M_{\text{IMF}} = 0$  and  $M_{\text{IMF}} \geq 5$  because the number of samples is small.

it almost reproduces them. The AMD-V results are  $M_p = 7.6$  and  $M_\alpha = 4.4$  while the data are  $M_p = 6.2$  and  $M_\alpha = 5.2$ .

Figure 7 shows the event-by-event analysis of the fragmentation pattern, such as the probability distribution of  $M_p$ ,  $M_\alpha$  and the IMF multiplicity  $M_{\text{IMF}}$ . The event-by-event correlation between  $M_{\text{IMF}}$  and  $M_p$  and that between  $M_{\text{IMF}}$  and  $M_\alpha$  are also shown. The degree of the reproduction by the usual AMD is similar to that by other models in Ref. [12], while the AMD-V result is much better than any other. Although  $M_p$  and  $M_\alpha$  have been almost reproduced by AMD-V, more  $\alpha$  particles and less protons should be produced in events with large  $M_{\text{IMF}}$  in order to get perfect results. We show in Fig. 8 the event-by-event distribution of the charge  $Z_{\text{max}}$  of the largest fragment versus the normalized second moment  $S'_2$  of the event charge distribution with the largest fragment excluded,

$$S'_2 = \sum_{i; Z_i \neq Z_{\text{max}}} Z_i^2 / \sum_{i; Z_i \neq Z_{\text{max}}} Z_i, \quad (32)$$

where  $i$  is the label of the fragments produced in an event. AMD-V again reproduces very well the experimental data shown in Fig. 12 of Ref. [12] in which there are two components, one with small  $S'_2$  and large  $Z_{\text{max}}$  and the other with large  $S'_2$  and small  $Z_{\text{max}}$ . The first

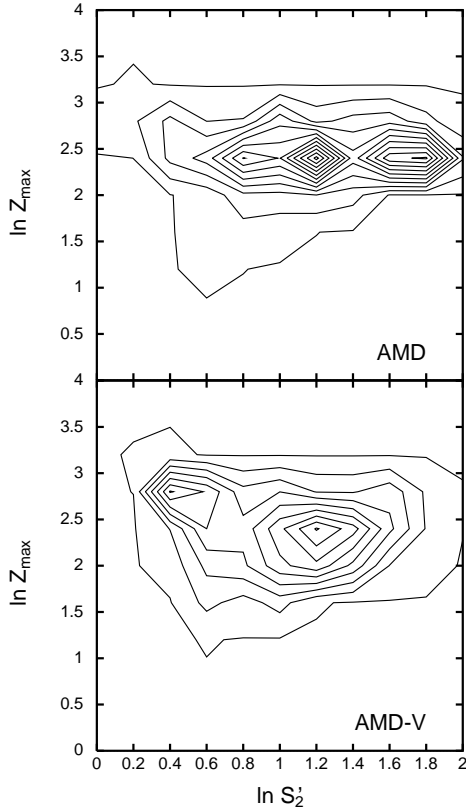


FIG. 8. Logarithmic distribution of  $Z_{\max}$  vs  $S'_2$  (see text). Each contour represents constant value of  $d^2P/d\ln S'_2 d\ln Z_{\max}$  where  $P$  is the probability normalized to 1. The outside contour is at a level of 0.01, and each inner contour represents a progressive increase of 0.15. Results of AMD (upper part) and AMD-V (lower part) are shown after the application of the experimental filter.

component corresponds to the events with a large IMF and many small fragments while the second component is due to the events with several IMFs produced. On the other hand, in the usual AMD result, the first component is missing because most events are binary. Binary events have produced a peak with too large  $S'_2$ .

The only unsatisfactory point of the AMD-V result in Fig. 6 is the underestimation of the multiplicity for  $Z = 3$  and 4. By investigating the time evolution of the system, we have found that light IMFs with  $5 \lesssim A \lesssim 10$  are often produced from time to time but they tend to merge with one another to form a larger fragment again. If this merging is spurious, we would get very good result by removing it, as shown in Fig. 9. In getting this result, we have assumed that the light IMFs with  $A \leq 13$  are put into the statistical decay code immediately after they are produced, unless they are absorbed by a large fragment with  $A \geq 14$  in later stage of the dynamical calculation. A possible reason why the merging of light IMFs may be spurious is that the diffusion and the splitting of the center-of-mass wave packets of clusters in a nucleus is not fully described in AMD-V when they are emitted from a nucleus. In AMD-V, the dispersion and the diffusion of the center-of-mass wave packet of a cluster is described through those of the nucleons contained in the cluster and therefore the diffusion of the center-of-mass wave packet is always accompanied by the internal excitation of the cluster. If the center-of-mass diffusion is treated separately from the internal degrees of freedom as it should be, more energy will be available for the translational kinetic energy of the cluster and the light IMF emission will increase. It should be noted that the zero-point

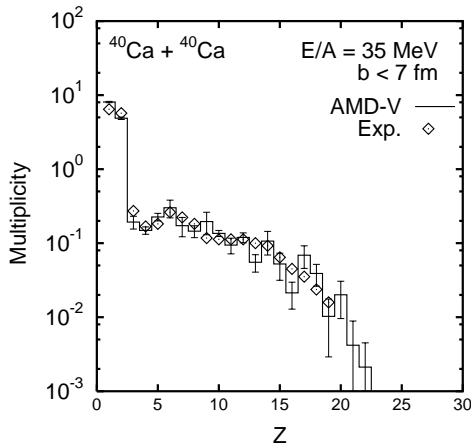


FIG. 9. The same as the lower part of Fig. 6 but the light fragments ( $A \leq 13$ ) are put into the statistical decay calculation immediately when they are produced after  $t = 150$  fm/c unless they are absorbed again by a heavy fragment ( $A \geq 14$ ) before  $t = 300$  fm/c.

oscillation energy per nucleon of the cluster center-of-mass motion is  $3\hbar^2\nu/2AM \approx 10/A$  MeV with  $A$  being the mass number of the cluster, and therefore it is less important for heavier clusters.

#### IV. RELATION OF AMD-V TO OTHER MODELS

In this section, we intend to clarify the interrelation among the frameworks of microscopic models which have been used for the study of the dynamics of heavy ion collisions, such as TDHF, VUU, QMD, AMD, and AMD-V. Since the nuclear reaction system is a quantum system and is described by a time-dependent wave function, we mainly discuss on the quantum models such as TDHF and AMD. However, most of the following discussions can be applied also to semiclassical models.

Before the discussion on the meaning of the newly introduced process of AMD-V, we will first mention on the difference of the treatments of two-nucleon collisions in one-body transport models and in molecular dynamics models. Let us take the initial state as a Slater determinant

$$|\Psi_0\rangle = \det[\psi_{01}\psi_{02}\cdots\psi_{0A}]. \quad (33)$$

In order to compare AMD with TDHF, we may take  $|\Psi_0\rangle$  to be an AMD wave function  $|\Phi(Z_0)\rangle$ . Here we consider  $|\Psi_0\rangle$  as the state just before the first chance of two-nucleon collision in a heavy ion reaction. If the first chance of two-nucleon collision happens between the first and the second nucleons, the wave function of these two nucleons changes as

$$\psi_{01}\psi_{02} \rightarrow \sum_{\alpha\beta} c_{\alpha\beta}\psi_1^{(\alpha)}\psi_2^{(\beta)}, \quad (34)$$

while other nucleon wave functions propagate as  $\psi_{0i} \rightarrow \psi_i$  ( $i = 3, \dots, A$ ) obeying the TDHF equation or some approximated equation.  $\alpha$  and  $\beta$  represent the single-particle states and one of the pairs of  $\alpha\beta$  corresponds to the state without two-nucleon collisions.

Accordingly, the initial Slater determinant has changed into a linear combination of many Slater determinants

$$|\Psi_0\rangle \rightarrow |\Psi\rangle = \sum_{\alpha\beta} c_{\alpha\beta} |\Psi^{(\alpha\beta)}\rangle, \quad (35)$$

$$|\Psi^{(\alpha\beta)}\rangle = \det[\psi_1^{(\alpha)} \psi_2^{(\beta)} \psi_3 \cdots \psi_A]. \quad (36)$$

Further successive two-nucleon collisions may cause more branching into Slater determinants. Since  $|\Psi\rangle$  is not a Slater determinant any more, TDHF cannot be applied to it. However, it should be noted that each component  $|\Psi^{(\alpha\beta)}\rangle$  is a Slater determinant and TDHF may be applied to it as a good approximation. Each  $\alpha\beta$  has its own mean field calculated from  $|\Psi^{(\alpha\beta)}\rangle$  and the single-particle wave functions propagate under this mean field. In order to decide the time evolution of a component  $|\Psi^{(\alpha\beta)}\rangle$ , no information of other components should be necessary because of the linearity of the quantum mechanics. However, what is done in one-body transport models like VUU and the extended TDHF for two-nucleon collisions strongly contradicts to this point of view. The extended TDHF (or VUU) calculates the effect of the two-nucleon collision on the one-body density matrix  $\rho(\mathbf{r}, \mathbf{r}')$  which can be always defined as

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \Psi | \hat{\rho} | \Psi \rangle, \quad \hat{\rho} = \sum_i |\mathbf{r}\rangle \langle \mathbf{r}'|_i, \quad (37)$$

though the system is not described by a single Slater determinant after the two-nucleon collision. The future time evolution of single-particle states is determined by the TDHF-like equation with the mean field calculated from  $\rho(\mathbf{r}, \mathbf{r}')$  as if it were not for any many-body correlation and as if the two-body density matrix could be given by an antisymmetrized product of two one-body density matrices. This means that the single-particle wave functions of all components  $|\Psi^{(\alpha\beta)}\rangle$  are propagated by a common mean field, which is in contradiction to the linearity of the time-dependent Schrödinger equation. On the other hand, in AMD (and many other molecular dynamics models), one of the components  $|\Psi^{(\alpha\beta)}\rangle$  is chosen stochastically as a channel with the probability  $|c_{\alpha\beta}|^2$  when a two-nucleon collision has happened. Here  $\alpha\beta$  may be considered as the scattering angle and  $c_{\alpha\beta}$  as the scattering amplitude. Namely, in AMD, the two-nucleon collisions are treated as the stochastic branchings into channels each of which is represented by an AMD wave function. Therefore the mean fields of different channels are different and the time evolutions of channels are independent of one another, which is a quite plausible feature. This is the reason why AMD is superior to the one-body transport models in the description of medium energy heavy ion collisions where the branching effect is more important than the flexibility of single-particle wave functions. A possible drawback of AMD treatment is that the effect of the two-nucleon collisions is treated stochastically by giving up the description of the interference among the components  $|\Psi^{(\alpha\beta)}\rangle$  after two-nucleon collisions.

The above-mentioned importance of the two-nucleon collision process as a source of the branching into channels should have been well known, and it is not directly related to the newly introduced process of AMD-V. Here we consider phenomena in which the two-nucleon collision process is not important, in order to clarify the relation and the difference among TDHF, AMD, and AMD-V. Let us take the Slater determinant  $|\Psi_0\rangle$  of Eq. (33) as

the initial state. For example,  $|\Psi_0\rangle$  may be an excited fragment produced in one of the channels of a medium energy heavy ion collision with  $A$  being the mass number of this fragment. It is usually sufficient to assume that  $|\Psi_0\rangle$  is equal to an AMD wave function  $|\Phi(Z_0)\rangle$  because AMD can describe the excited fragments in good approximation. According to TDHF equation, the single-particle wave functions will propagate for a short period, and the many-body wave function will change as

$$|\Psi_0\rangle \rightarrow |\Psi\rangle = \det[\psi_1\psi_2\cdots\psi_A]. \quad (38)$$

Now let us consider the case in which the first nucleon is going out of the nucleus with some probability while the others remain in it. (It is trivial to generalize the following discussion to the case in which all nucleons can be emitted.) Then the propagated single-particle wave function of the first nucleon can be decomposed into two (or more) parts as

$$\psi_1 = \sum_{\alpha} c_{\alpha} \psi_1^{(\alpha)}, \quad (39)$$

where  $\psi_1^{(1)}$  is spatially localized in the nucleus and  $\psi_1^{(2)}$  is out-going part of  $\psi_1$ . Accordingly, the Slater determinant  $|\Psi\rangle$  can be written as a linear combination of two (or more) Slater determinants as

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\Psi^{(\alpha)}\rangle, \quad (40)$$

$$|\Psi^{(\alpha)}\rangle = \det[\psi_1^{(\alpha)}\psi_2\cdots\psi_A]. \quad (41)$$

Then, in order to solve the further time evolution of  $|\Psi\rangle$ , we can think of two different ways. The first way is to continue solving TDHF equation for  $|\Psi\rangle$  of Eq. (38) as is widely done in TDHF calculation. The second way is to apply TDHF equation to each Slater determinant  $|\Psi^{(\alpha)}\rangle$  and solve the time evolution of each channel independently. Of course, these two ways are equivalent for the exact quantum mechanics due to the principle of superposition. However, it is not true for the approximated treatment like TDHF where the nonlinearity has been introduced for the sake of the feasibility of calculation. The first way corresponds to using the common mean field to all channels of Eq. (40), while the mean fields for  $|\Psi^{(\alpha)}\rangle$  are different from channel to channel in the second way. Which way should we take for the best description of the system? It should be noted that  $|\Psi^{(1)}\rangle$  represents a nucleus of mass number  $A$  with all nucleons spatially localized in the nucleus, while  $|\Psi^{(2)}\rangle$  is equivalent to the product of the state of a nucleus with mass number  $A - 1$  and the state of the out-going nucleon. Therefore we can say, at least, that the second way is reliable as long as the TDHF description of nuclei with mass numbers  $A$  and  $A - 1$  is reliable. On the other hand, in the first way, the common mean field for all channels is made by fractional number of nucleons between  $A - 1$  and  $A$ , and such mean field cannot be a good one for the nucleus with mass number  $A - 1$  nor  $A$ . Although this pathological nature of TDHF for nucleon emission may not be so serious in practice, this example explains how the breakdown of the usual TDHF begins to grow up into the nonsense description of the multichannel final state in heavy ion collisions even when the two-nucleon collision effect is not directly important. From this consideration, we can adopt an approximation that, when

single-particle wave functions are spreading wide like in the case of nucleon emission, a Slater determinant should be decomposed into a linear combination of channel Slater determinants by decomposing single-particle wave functions into localized components and then the time evolutions of channel Slater determinants should be solved separately to get reliable results in the global time scale.

Now let us consider the case of AMD. It should be noted first that the TDHF result  $|\Psi\rangle$  of Eq. (38) is more reliable than the AMD result  $|\Phi(Z_0)\rangle \rightarrow |\Phi(Z)\rangle$  for the time evolution of a short period because the TDHF single-particle wave function is more general than that of AMD. When the nucleon-emission channel  $|\Psi^{(2)}\rangle$  is a minor branch, the AMD equation of motion will simply abandon this channel and  $|\Phi(Z)\rangle$  will be almost equivalent to  $|\Psi^{(1)}\rangle$ . Although the loss of minor channels is not satisfactory, the time evolution of the main channel will be described rather well just as in the second way of the previous paragraph because the pathological situation of TDHF will not occur in AMD due to the compact single-particle wave functions.

The meaning of the newly introduced process of AMD-V is now quite obvious. At first the system is represented by an AMD wave function  $|\Psi_0\rangle = |\Phi(Z_0)\rangle$  and its time evolution for a short period is calculated with TDHF (or Vlasov) equation. Each single-particle wave function may begin to spread. Then it is decomposed as in Eq. (39) with  $\psi_1^{(\alpha)}$  being Gaussian wave packets. Accordingly, the many-body wave function is decomposed as in Eq. (40) into many AMD wave functions  $|\Psi^{(\alpha)}\rangle$  in this case. One of these channels  $|\Psi^{(\alpha)}\rangle$  is chosen with the appropriate probability and its future time evolution is solved just in the same way as was done for  $|\Psi_0\rangle$  without any influence from other channels. Thus AMD-V respects the minor channels which are lost in AMD. It should be emphasized that TDHF (or Vlasov) equation is always applied to the instantaneous time evolution of an AMD wave function with compact single-particle wave functions and therefore AMD-V is free from the pathological nature of TDHF that would appear for a Slater determinant which should be decomposed into channels. In principle, the best way among the arbitrary ways to decompose a Slater determinant is to decompose the Slater determinant into channel Slater determinants so that the future time evolutions of all the channels can be calculated most precisely in mean field approximation. The important standpoint of AMD-V is therefore to take the AMD wave functions as the channel wave functions to which TDHF equation can be applied most safely.

It should be commented that in the above explanation of AMD-V we have ignored the interference among channels  $|\Psi^{(\alpha)}\rangle$ . Generally speaking, it is very difficult to respect the interference because the time evolutions of all channels should be calculated very precisely in the global time scale in order to get meaningful results with interference. This difficulty is avoided in AMD-V by introducing semiclassical treatments by using Vlasov equation instead of TDHF equation and QMD-like representation of the one-body distribution function instead of the AMD wave function. In other words, we have replaced the many-body density matrix of a pure state  $|\Psi\rangle$  with a statistical ensemble of channel wave functions  $|\Psi^{(\alpha)}\rangle$  as

$$|\Psi\rangle\langle\Psi| = \sum_{\alpha\beta} c_\alpha c_\beta^* |\Psi^{(\alpha)}\rangle\langle\Psi^{(\beta)}| \approx \sum_{\alpha} w_\alpha |\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|, \quad (42)$$

where the probability  $w_\alpha$  of branching is decided so that Vlasov equation is reproduced as much as possible. The energy recovery procedure explained in Sec. II.B.3 ensures that

the channels can be physical when they have evolved into the final state. The limitation of channel wave functions  $|\Psi^{(\alpha)}\rangle$  to AMD wave functions is essential in many senses. As already discussed, the mean field approximation can be applied to the AMD wave functions more safely than to general Slater determinants. Furthermore, AMD wave functions agree with the intuitive concept of ‘events’ that the system is divided into moving fragments composed of integer number of nucleons in each event. Since one usually does not think of an observable that connects different events (or channels), the interference terms in Eq. (42) are usually irrelevant. Only for the internal motions in a fragment, the interference may be important when one is interested in the precise single-particle wave functions. It should be finally emphasized that we still have many-body wave functions  $|\Psi^{(\alpha)}\rangle$  which have quantum mechanical information within channels, in spite of the semiclassical treatment of branching introduced to respect the independence among channels which is also an important quantum mechanical feature.

## V. SUMMARY

In this paper, we have presented a new version of AMD with stochastic incorporation of Vlasov equation. In this AMD-V, the diffusion of wave packets according to Vlasov equation is treated as the stochastic branching into events. Namely, in addition to the equation of motion and two-nucleon collisions of the usual AMD, stochastic displacements are given to the centroids of wave packets so as to reproduce the time evolution of one-body distribution function predicted by Vlasov equation. No important free parameters are introduced for this new process of AMD-V. The mean fields are different from event to event, and therefore the independence among the time evolutions of events (or channels) is treated properly unlike the TDHF (or Vlasov) calculation. It should be noted that at any time of each event we have an AMD wave function to which Vlasov equation is applied. The merit of this fact is not only that the mean field can be calculated easily but also that the mean field approximation can be adopted more safely than for a general Slater determinant which may have to be treated as a linear combination of several channels. AMD-V is a fully quantum mechanical framework with channel wave functions except that the interference among channels cannot be calculated. However, the extension of AMD-V is not directly related to the exact antisymmetrization in AMD and therefore this extension is applicable to other molecular dynamics models with wave packets. Although we have introduced AMD-V as an extension of AMD to remove the restriction on the shape of wave packets, it is also possible to regard AMD-V as giving a scheme to extend the TDHF (or Vlasov) calculation to go beyond a Slater determinant by taking account of the branchings into channels and respecting the independence among them.

The ability of AMD-V to describe the fragmentation in medium energy heavy ion collisions has been demonstrated by the very good reproduction of data for  $^{40}\text{Ca} + ^{40}\text{Ca}$  system at 35 MeV/nucleon, which have never been reproduced by any other model. The new stochastic process of AMD-V has enabled the description of minor branching processes which are irrelevant to the two-nucleon collision process, such as the evaporation of nucleons from a hot nucleus and the nucleon transfer in heavy ion collisions. In the case of  $^{40}\text{Ca} + ^{40}\text{Ca}$  system at 35 MeV/nucleon, the spurious binary feature of the AMD result has been removed by



AMD-V and the abundant production of light IMFs and  $\alpha$  particles is described very well mainly as the result of the formation of neck region between projectilelike and targetlike components which have passed through each other with dissipation. Produced fragments are already cool and the statistical decay calculation is not so important as in the case of AMD.

The proposition of AMD-V has derived from our study of the statistical property of AMD. The successful description of fragmentation in heavy ion collisions can also be interpreted as due to the improvement of the statistical property. Namely, the improvement of the caloric curve to the quantum mechanical one is important to reduce the excitation energy of fragments. Furthermore, the pressure (i.e., the force necessary to keep the volume) of the hot nuclear matter has been increased by the new process of AMD-V, which facilitates the expansion of the hot system followed by the fragmentation. However, what should be emphasized here is that such an improvement is just a straightforward result of the improvement of the microscopic single-particle dynamics to enable the diffusion of wave packets.

AMD-V adopts Vlasov equation for the instantaneous time evolution of the AMD wave function. Although this mean field approximation seems to have given very satisfactory results of fragmentation, there still remains some underestimation of data for the yield of Li and Be isotopes in  $^{40}\text{Ca} + ^{40}\text{Ca}$  system at 35 MeV/nucleon. A possible solution of this problem will be the proper treatment of the center-of-mass motions of clusters in a nucleus. Namely the diffusion of the center-of-mass wave packet of a cluster, which often appears in the fragmenting system, should be treated separately from the diffusion of the wave packets of internal degrees of freedom of the cluster. Such extensions will be made in the future work.

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